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# An orbital antiferromagnetic state in the extended Hubbard model

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**Abstract** : Ground states of an orbital antiferromagnetic order, along with the charge density waves and spin density waves, are considered within the framework of an extended Hubbard model The model includes nearest neighbour ($-t$) and next nearest neighbour ($t'$) hopping matrix elements as well as on-site ($U$) and nearest neighbour ($V$) repulsions between fermions Ground state phase diagram of the model is calculated within the Hartree-Fock approximation For $t' = 0$, only charge and spin density waves are stable For non-zero $t'$, the orbital antiferromagnetic order, characterised by $d_{x^2-y^2}$ symmetry, is stable over a finite portion of the phase diagram, which grows in size with increasing $t'$

**Keywords** : Ground state phase diagram, particle-hole ordering, staggered flux phase

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The high temperature superconductors (HTS) are doped cuprates of lanthanum, yttrium, bismuth, thallium *etc.* and are predominantly characterised by their strange normal state properties. The parent materials (without doping) are found to be antiferromagnetic insulators [1] contrary to the conclusions from the band structure calculations [2], according to which these are metals. This behaviour as well as their strange properties with doping, are believed to arise due to the strong electronic correlations present. In addition, properties of these cuprates are found to be dominated by $CuO_2$ plane. Hence Hubbard model in two dimension could be an usefull starting point. In fact, Hubbard model and its different extended or strong coupling versions are extensively studied in the recent years, in connection with the cuprate superconductors, and systems with strong correlations in general. Phase diagrams of such models are thus of inherent interest. In this communication, we study the ground state phase diagram of an extended Hubbard model focussing on the stability of an orbital antiferromagnetic state.

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The Hamiltonian of the extended Hubbard model on a square lattice, is given by $H = H_0 + H_I$,

$$H_0 = \sum_{k,\sigma} (\xi_k - \mu) c^{\dagger}_{k,\sigma} c_{k,\sigma} \tag{1a}$$

and

$$H_I = U \sum_{i} \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow} + \frac{V}{2} \sum_{i,\sigma,\sigma'} \sum_{\delta_{nn}} \hat{n}_{i,\sigma} \hat{n}_{i+\delta_{nn},\sigma'} \tag{1b}$$

where $c^{\dagger}_{k,\sigma}(c_{k,\sigma})$ creates (annihilates) a fermion with momentum $k$ and spin $\sigma$, $n_{i,\sigma}$ are number operators, $\mu$ is the chemical potential and $\delta_{nn} = \pm a\hat{x}, \pm a\hat{y}$ are nearest neighbour lattice vectors with $a$ being the lattice constant. The interactions are on-site ($U$) and nearest neighbour ($V$) repulsions and independent of lattice sites. The band dispersion, comprising of nearest neighbour ($-t$) and next nearest neighbour ($t'$) hopping matrix elements, is given by $\xi_k = -t\big(\cos(k_x a) + \cos(k_y a)\big) + t' \cos(k_x a) \cos(k_y a)$. For $t' = 0$ and at half filling, the Fermi surface (FS) is perfectly nested $\xi_{k+Q} = -\xi_k$, where $Q = (\pi, \pi)$ is the nesting vector. With the nested FS and for $V = 0$, the ground state Hartree-Fock, particle-hole ordering is a two sublattice spin density wave (SDW) for small $U$ Detailed random phase approximation (RPA) studies [3] of the collective excitation spectrum have shown that this is the case even at large $U$. Introduction of $V$ induces a charge ordering in the form of charge density waves (CDW) [4], which is energetically favoured to SDW for $V > U/4$.

It was first noted by Halperin and Rice [5] that, particle-hole ordering can produce ground states other than CDW and SDW. One such is an orbital antiferromagnetic (OAF) state. The OAF state arises out of a $d$-wave particle-hole pairing, that gives rise to circulating charge currents in the square lattice with the orientation of the circulation being opposite in the neighbouring elementary plaquettes [6]. This is, thus similar to the staggered flux phase studied earlier [7] as a possible ground state of the $t$-$J$ model. The $d$-wave particle-hole pairing, involved in the formation of the OAF state, is interesting in the light of a pseudo-gap found in the underdoped cuprates by photoemission experiments [8,9], where the gap function has a $d_{x^2-y^2}$ symmetry. Within the extended Hubbard model, OAF state was discussed earlier [10,11] giving vent to the speculations that this might be stable compared to CDW and SDW ground states if the nesting of FS is removed [6]. However, no attempt has been made to establish its stability compared to the CDW and SDW, which is the principal focus of the present communication. We do a Hartree-Fock analysis of the ground states of different particle-hole orderings such as CDW, SDW and OAF, and obtain the ground state phase diagram for the half filled band [12].

Mean-field decoupling of the Hamiltonian in eqn. (1) enables one to have the CDW order parameter (in the real space) of the form

$$\langle \hat{n}_{i,\sigma} \rangle = \frac{1}{2} + \frac{p}{2} \cos(\boldsymbol{Q}.\boldsymbol{R}_i) \tag{2}$$

and the SDW state (considering a z-polarized state) is defined as

$$\left\langle \hat{n}_{i,\sigma} \right\rangle = \frac{1}{2} + \sigma \frac{m}{2} \cos(\boldsymbol{Q}.\boldsymbol{R}_i) \tag{3}$$

where $p$ amd $m$ are the amplitudes of the induced charge and spin density modulation respectively and $\sigma = +1$ $(-1)$ for up (down) spins. The OAF state has non-zero intersite averages

$$\left\langle c^{\dagger}_{i,\sigma} c_{i\pm\hat{i}\sigma} \right\rangle = ig\cos(\boldsymbol{Q}.\boldsymbol{R}_i) \tag{4a}$$

and

$$\left\langle c^{\dagger}_{i,\sigma} c_{i\pm\hat{j}\sigma} \right\rangle = -ig\cos(\boldsymbol{Q}.\boldsymbol{R}_i) \tag{4b}$$

Substitution of the mean field values from eqns. (2–4), yields a mean-field decoupled Hamiltonian from eqn. (1) as

$$H^{s}_{MF} = \sum_{k,\alpha}^{RBZ} \left[ (\xi_k - \mu) c^{\dagger}_{k,\alpha} c_{k,\alpha} + (\xi_k + Q - \mu) c^{\dagger}_{k+Q,\alpha} c_{k+Q,\alpha} \right] + \sum_{k,\alpha,\beta}^{RBZ} \left[ (\Delta^{s}_{\alpha,\beta}(k) c^{\dagger}_{k,\alpha} c_{k+Q,\beta} + h.c \right] + X_s \tag{5}$$

The reduced Brillouin zone (RBZ) is due to the modulation by $\boldsymbol{Q}$, which effects a folding up of the original Brillouin zone. Here $\Delta^{s}_{\alpha,\beta}(k)$ is the generalized order parameter with $s = 1$, 2 and 3 corresponding to CDW, SDW and OAF states respectively. Thus,

$$\Delta^{1}_{\alpha,\beta}(k) = \delta_{\alpha,\beta}\left(\frac{U}{2} - 4V\right)p \qquad \text{for the CDW state} \tag{6a}$$

$$\Delta^{2}_{\alpha,\beta}(k) = \delta^{z}_{\alpha,\beta}\left(-\frac{U}{2}\right)m \qquad \text{for the z-polarized SDW state} \tag{6b}$$

$$\Delta^{3}_{\alpha,\beta}(k) = i\delta_{\alpha,\beta}(\cos k_x - \cos k_y)(-2V)g \qquad \text{for the OAF state} \tag{6c}$$

where $\sigma^z$ is a Pauli matrix. The constant part $X_s$ (in eqn. (5)) for different states are, $X_1 = (2V - U/4)p^2N$, $X_2 = (U/4)m^2N$ and $X_3 = 4Vg^2N$, where $N$ is the total number of sites. In eqn. (5) we suppress writing the factor $(U/2 + 4V)$ for each state and absorb it in the chemical potential. In $X_s$ also, we ignore the contribution $-(U/4 + 2V)N$ for each state, which shifts the ground-state energies by equal amount.

The mean field Hamiltonian of eqn. (5) is diagonalized by a canonical transformation. The folding of the Brillouin zone results in the formation of two bands

$$e^{(+)}_{s}(k) = (\eta_k - \mu) + \sqrt{\varepsilon^2_k + \Delta^2_s(k)} \tag{7a}$$

and

$$e^{(-)}_{s}(k) = (\eta_k - \mu) - \sqrt{\varepsilon^2_k + \Delta^2_s(k)} \tag{7b}$$

where $\Delta_1(k) = (U/2 - 4V)p$, $\Delta_2(k) = -(U/2)m$ and $\Delta_3(k) = -2Vg(\cos(k_x a) - \cos(k_y a))$. It is clear that CDW ($\Delta_1(k)$) and SDW ($\Delta_2(k)$) states are isotropic ($s$-wave) whereas the OAF

state ($\Delta_3(k)$) has order parameter of $d_{x^2-y^2}$ symmetry. Here $\eta_k = (\xi_k + \xi_{k+Q})/2$, $\varepsilon_k = (\xi_k - \xi_{k+Q})/2$. For $t' = 0$, one has $\eta_k = 0$, enforcing the nesting of the Fermi surface. This also implies that $\mu = 0$ and the lower band $e_k^{(-)}$ is completely full whereas the upper band $e_k^{(+)}$ is completely empty. However for nonzero $t'$, $\eta_k \neq 0$, nesting of the Fermi surface is removed at half filling, and the overlapping of bands is possible.

The self-consistent equations for the chemical potential $\mu$ and the order parameters are

$$\frac{1}{2} = \frac{1}{N}\sum_{k}^{RBZ}\left[\Theta\left(-e_\gamma^{(-)}(k)\right) + \Theta\left(-e_s^{(+)}(k)\right)\right] \tag{8a}$$

and

$$\frac{1}{\Gamma_\gamma} = \frac{2}{N}\sum_{k}^{RBZ}\frac{\omega_k^s\left[\Theta\left(-e_s^{(-)}(k)\right) - \Theta\left(-e_s^{(+)}(k)\right)\right]}{\sqrt{\varepsilon_k^2 + \Delta_s^2(k)}} \tag{8b}$$

where $\Gamma_1 = 4V - U/2$, $\Gamma_2 = U/2$, $\Gamma_3 = V/2$ and $\omega_k^s$ is the symmetry factor of the order parameters with $\omega_k^1 = \omega_k^2 = 1$ (for SDW and CDW) and $\omega_k^3 = [\cos(k_x a) - \cos(k_y a)]^2$ (for OAF).

Expression for the ground state energy (per site) turns out to be

$$E^s = \frac{X_\gamma}{N} + \frac{2}{N}\sum_{k}^{RBZ}[e_s^{(-)}(k)\Theta(-e_\gamma^{(-)}(k)) + e_s^{(+)}(k)\Theta(-e_s^{(+)}(k))] \tag{9}$$

Self consistent equations (8) are solved numerically to obtain the values of $\mu$ and gap function $\Delta_\gamma(k)$, which are then used to evaluate the ground state energies $E_\gamma$ in eqn. (9). In

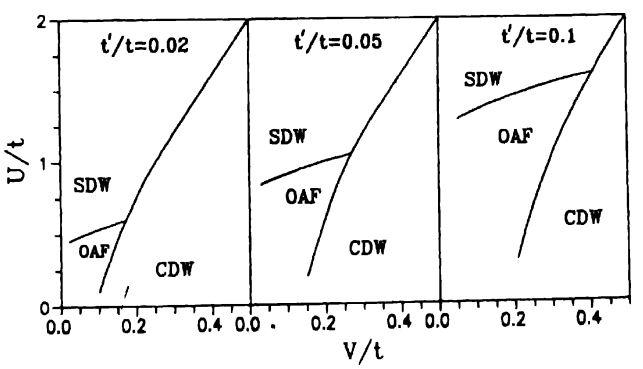


**Figure 1.** The mean-field phase diagram of the extended Hubbard model, as obtained by comparison of the ground state energies of the states considered. The region of stability of the OAF state grows with increasing $t'/t$ ratio, as is evident in the figure. The phase boundaries for small values of $U/t$ and $V/t$ are not shown since numerical difficulties prevented an accurate determination of their positions.

Figure 1 we present the ground state phase diagram in the ($U/t$, $V/t$) plane, for different values of parameter $t'/t$. For $t' = 0$, the CDW and SDW states are only stable and are

separated by a phase boundary at $U = 4V$ (not shown). Any nonzero $t'$ results in the destruction of nesting of the FS and thereby helps to stabilize the OAF state at weak coupling.

The gap functions in the CDW, SDW and OAF states are proportional to $4V - U/2$, $U/2$ and $2V$ respectively. Thus the OAF state is expected to be energetically close to the other two states near the $U = 4V$ line. In fact, for the perfectly nested FS ($t' = 0$), the OAF state becomes degenerate with the CDW and SDW at weak couplings on the $U = 4V$ line [13]. At large $U$, the minimization of the double occupancy in the ground state is achieved by the SDW ordering with $m \to 1$, whereas for large $V$ the energy cost associated with having electrons on neighbouring sites could be avoided through a CDW ordering with $p \to 1$. Thus the OAF state is expected to arise only at weak coupling and close to the $U = 4V$ line. Although a physical interpretation of the fact that, introduction of $t'$ stabilizes the OAF state, is not possible at this stage, our results suggest that the OAF state is more robust for the case of a non-nested Fermi surface. This is interesting since real materials often have non-nested Fermi surface.

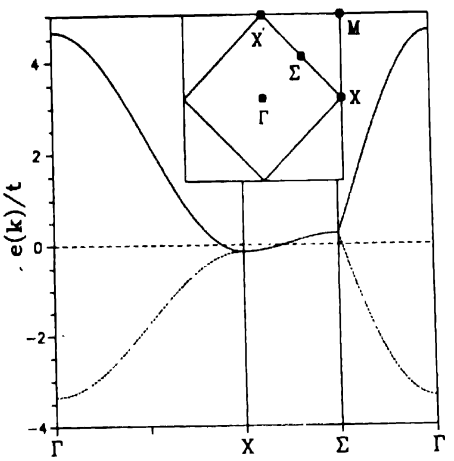


**Figure 2.** Quasiparticle dispersion energy $e_k^{(+)}$ and $e_k^{(-)}$ for the OAF state along the symmetry directions of the reduced Brillouin zone, shown explicitly in the inset. The solid curve $e_k^{(+)}$ corresponds to the conduction band while the dashed curve $e_k^{(-)}$ is for the valence band. The parameters are $t'/t = 0.1$, $U/t = 1.5$ and $V/t = 0.37$ for which the OAF state is stable

To understand the material characteristic of the OAF state, we plot in Figure 2, the dispersion $e_k^{(-)}$ and $e_k^{(+)}$ (for the OAF state) as a function of $k$, for nonzero $t'/t$, with $U/t$ and $V/t$ chosen to ensure the stability of the OAF state. The overlapping of bands implies that the valence band is not completely full and the conduction band is not completely empty and the density of states at Fermi surface is found to be suppressed but nonzero. The OAF state is therefore a poor metallic state with a pseudogap at the Fermi surface.

It should be memtioned here that, a circulating spin current along the elementary plaquettes of the square lattice, could produce a spin nematic (SN) order [11,14]. Within the

Hartree-Fock approximation, the SN state is degenerate with the OAF state and has indentical $e_k^{(+)}, e_k^{(-)}$ bands, although physically these states are quite different. The OAF state originates out of circulating charge currents which produce staggered orbital magnetic moments in the elementary plaquettes, whereas the SN state is due to the circulating spin currents. Thus, though a magnetic neutron scattering experiment could differentiate between OAF and SN states, they will appear identical to any experiment probing only their band structures or single particle properties.

To summarize, we have obtained the ground state (zero temperature) phase diagram of the extended Hubbard model on a square lattice at half-filling showing relative stability of the competing orders of CDW, SDW and OAF states. We find that for nonzero values of $t'$, the OAF state is favourable to the SDW and CDW states, over a finite range of parameters in the weak coupling region. The size of this region, where OAF state is stable, increases with increasing $t'$.

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